

Ethanimidic acid, N-hydroxy-, ethyl ester  
10576-12-2 | DTXSID2065129

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

## Model Results

**Predicted value:**  $2.23\text{e-}12 \text{ cm}^3/\text{molecule}\cdot\text{sec}$

**Global applicability domain:** Inside

**Local applicability domain index:**  $5.21\text{e-}01$

**Confidence level:**  $8.09\text{e-}01$

## Nearest Neighbors from the Training Set

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N-Butylnitrite

**Measured:**  $2.72\text{e-}12$

**Predicted:**  $1.86\text{e-}12$

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Butyl nitrate

**Measured:**  $1.71\text{e-}12$

**Predicted:**  $1.60\text{e-}12$

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Isobutyl nitrate

**Measured:**  $9.20\text{e-}13$

**Predicted:**  $1.33\text{e-}12$

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1-Nitrobutane

**Measured:**  $1.50\text{e-}12$

**Predicted:**  $1.21\text{e-}12$

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N-Methylcarbamic acid, ethyl ester

**Measured:**  $8.30\text{e-}12$

**Predicted:**  $1.01\text{e-}11$